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THE MOBILITY OF NON-PLANAR DISLOCATIONS AHEAD OF A CRACK TIP

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ABSTRACT

In this paper, we first show using a generalised Peierls-Nabarro dislocation model that, if the cause of the low mobility of a dislocation is due to the need to transform the core from a non-planar configuration to a planar one, then this transformation will be greatly enhanced in the vicinity of a crack tip. The physical reason is that, being a free surface, the presence of the crack tip will reduce the mechanical rigidity of the matrix in which the dislocation is situated. We then present atomistic simulation results on screw dislocations in iron to show that this mobility enhancement effect is indeed a real one. The results suggest that there exists a critical stress intensity factor K_{mc} of the order of ~ 0.15 $\mu\sqrt{b}$ (μ = shear modulus, b = Burgers vector), such that if the applied stress intensity factor is larger than this value, all dislocations ahead of the crack tip would be planar and mobile. K_{mc} is found to be lower than the critical stress intensity factor for nucleation from crack-tip, and so crack-tip emission is nucleation rather than mobility controlled.

KEYWORDS

Dislocation, crack-tip plasticity, atomistic simulation, brittle-to-ductile transition

INTRODUCTION

The brittle-to-ductile transition (BDT) has been a problem of considerable practical and theoretical interest. It is generally believed that BDT will occur when dislocation sources near the crack tip can send out dislocations quick enough to shield the crack tip [1], or when dislocations can emanate quick enough from the crack tip itself to shield or blunt it. In the latter case, Weertman [2], Schoeck [3,4], Rice [5,6], and Xu et al [7] have investigated the problem of dislocation emission from crack tips. In their work, the process of gradually forming a dislocation from zero to unit Burgers vector content is considered in detail, and the relative ease of dislocation nucleation in competition with crack cleavage is studied. In the incipient process considered by these authors, the dislocation is assumed to have a planar core. In particular in Rice's model, a *J*-integral was used to evaluate the fault energy change as the dislocation forms from the crack tip. This results in the model's inability to account for any lattice friction that might act on the dislocation during the incipient process. In materials exhibiting the BDT, the intrinsic Peierls

stress is high and so lattice friction should not be neglected *a priori* in a satisfactory treatment on crack-tip plasticity.

In the present paper we focus on the interaction between the ½<111> screw dislocation and a mode III crack tip in the body-centred cubic (BCC) structure. The ½<111> screw dislocation has a three-fold non-planar core and is therefore representative of a system with a large friction stress. We will first use a semi-continuum approach based on a generalised version of the Peierls-Nabarro model [8] which can cater for non-planar dissociation of the dislocation core. This is then followed by atomistic simulation which serves to verify the conclusions reached by the semi-continuum model.

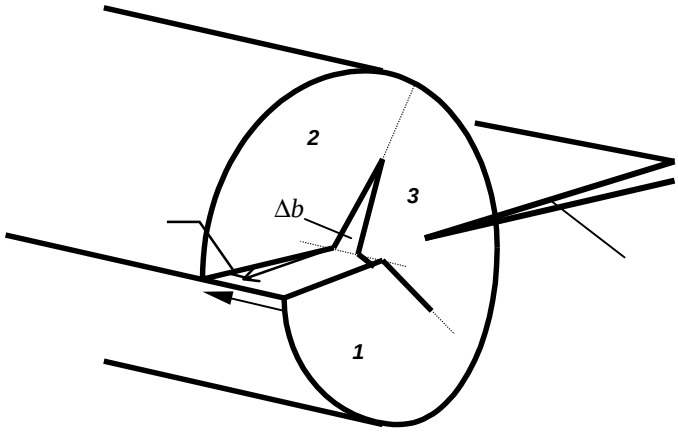

Figure 1: Three-fold screw dislocation ahead of a mode III crack tip

SEMI-CONTINUUM MODEL

In the generalised Peierls-Nabarro model, the ½<111> screw dislocation is modelled as elastically strained wedges joined together at surfaces parallel to the dislocation line over which atomic misfit takes place (Figure 1). The force law operating across the misfit surfaces is non-linear and may be assumed to have a simple Frenkel form

$$\gamma = \frac{\mu b}{4\pi^2}\left[1-\cos\left(\frac{2\pi\Phi}{b}\right)\right], \tag{1}$$

where μ is the shear modulus, b the Burgers vector and Φ the misfit displacement. When the screw dislocation is situated at a distance x ahead of a mode III crack tip, the total energy E_{tot} may be expressed as

$$\begin{aligned} E_{tot} = {} & \frac{3\mu}{2\pi}\int_0^\infty\int_0^\infty \{\frac{2\eta^2}{(\eta^3-\xi^3)}\sqrt{\frac{\xi^3+x^3}{\eta^3+x^3}}\,u_{3-}'(\xi)u_{3-}(\eta) + \frac{\sqrt{\eta}}{\eta^{3/2}+\xi^{3/2}}\left[u_{2-}'(\xi)u_{2+}(\eta)+u_{2+}'(\xi)u_{2-}(\eta)\right] \\ & + \frac{\sqrt{\eta}}{\eta^{3/2}-\xi^{3/2}}\left[u_{2+}'(\xi)u_{2+}(\eta)+u_{2-}'(\xi)u_{2-}(\eta)\right]\}\,d\eta\,d\xi \\ & + 2\int_0^\infty \gamma[\Phi=\Delta b-u_{3-}(r)-u_{2+}(r)]\,dr + \int_0^\infty \gamma[\Phi=(1-2\Delta)b-2u_{2-}(r)]\,dr \\ & - 2\int_0^\infty \tau_c(r)[u_{3-}(r)+u_{2+}(r)]\,dr + 2\int_0^\infty \frac{K_{III}}{\sqrt{2\pi(r+x)}}u_{2-}(r)\,dr \end{aligned} \tag{2}$$

where K_{III} is the applied stress intensity factor and $\tau_c(r) = K_{III}\cos(\psi/2+\pi/3)/\sqrt{2\pi\rho}$, $\rho=\sqrt{r^2+x^2-rx}$, $\psi = \tan^{-1}[\sqrt{3}r/(2x-r)]\in[0,\pi]$. In this expression, the double integral term is the strain energy, the

terms involving γ the misfit energy and the last two terms the work-done against applied stress. $u_{i\pm}(r)$ is the displacement function of the boundary marked by + or - of wedge *i* relative to the wedge tip position (see Figure 1). Δ is the Burgers vector content of the misfit surface 2|3 or 3|1, and can be used as a parameter specifying the degree of recombination of the core into the planar state. In the absence of the crack-tip, the core configuration should be symmetrically three-fold, and Δ will assume the value 1/3, and when the core is totally constricted into the planar state, Δ will become 0. The boundary displacements are subject to $u_{3-}(0) = 0$, $u_{3-}(\infty) = b/2$, $u_{2-}(0) = 0$, $u_{2-}(\infty) = (1/2-\Delta)b$, $u_{2+}(0) = 0$, $u_{2+}(\infty) = (\Delta-1/2)b$ because of the necessity to match with the Volterra solution in the long-range.

The stable configurations of the dislocation core under various conditions were obtained by minimising E_{tot} in eqn. (2) with respect to Δ, u_{3-}, u_{2+} and u_{2-} by variational means. More details about the methodology used are given in ref. [9]. Figure 2 shows the relation between the fractional Burgers vector Δ and the applied load at different values of distance *x* between the dislocation and the crack tip. It can be seen that with increasing stress, Δ initially decreases gradually. However, as soon as Δ decreases beyond ~ 0.25, the conversion towards the planar configuration speeds up quickly, implying that as long as the Burgers vector content in the 1|2 branch parallel to the crack plane reaches about 0.5, the core transforms very quickly to the planar state. As comparison, the behaviour of the screw core without the presence of the crack tip has also been investigated by Ngan [8,9]. In this case, the total energy functional is simpler than that shown in eqn. (2) but because of limitation of space it is not reproduced here. Figure 3 shows the relation between the fractional Burgers vector Δ and the stress applied along the Burgers vector on the 1|2 plane. It can be seen that Δ drops gradually with increasing stress and a rapid transformation to the planar state at $\Delta \approx 0.25$ does not occur in the crack-free situation. The rapid transformation to the planar state at $\Delta \approx 0.25$ in the presence of the crack in Figure 2 can be understood from the γ force law expressed in eqn. (1), in which the misfit energy attains a maximum when Φ equals 0.5*b*. Thus as soon as the tip of the 1|2 branch opens by more than 0.5*b*, corresponding to Δ falling below 0.25, the misfit force law exerts a force trying to enlarge the opening along the 1|2 branch. In the absence of a crack, the enlargement of branch 1|2 is resisted by the associated strain energy rise mainly in wedge 3 and so no instability situation arises. However, if wedge 3 is cracked as shown in Figure 1, it will become much less rigid and so the misfit energy may prevail. To prove that $\Delta \approx 0.25$ indeed marks an instability point in the cracked situation, stress removal tests were performed. It was found that if the core is stressed to any configuration with $\Delta > 0.25$, the configuration will return to the stress-free stable configuration upon removal of the applied load. However, if the core is stressed to beyond the $\Delta \approx 0.25$ point so that it has become planar, then upon removal of stress, the core will remain in the planar configuration with $\Delta \approx 0$. This shows that the planar state is a metastable state.

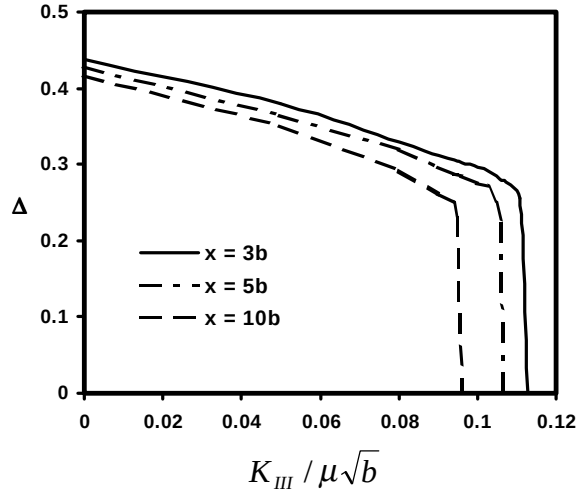

Figure 2: Core behaviour ahead of crack tip

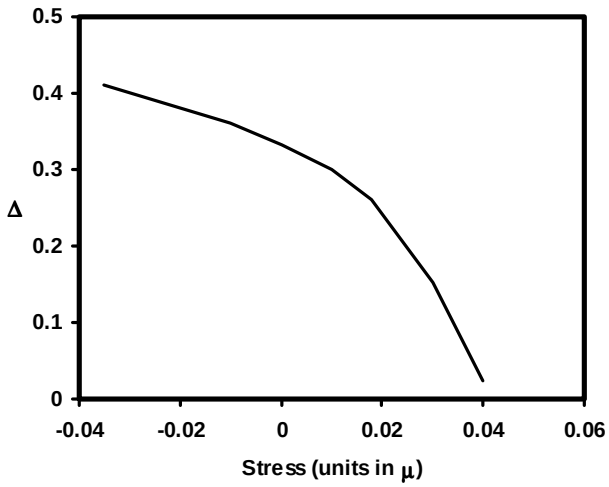

Figure 3: Core behaviour in bulk crystal

The above results suggest that the mobility of the screw dislocation is greatly enhanced ahead of a crack tip. To estimate the effective Peierls stress τ_p in the presence of a crack tip, we write

$$\frac{K_m}{\sqrt{2\pi x}} = \tau_p + \frac{\mu b}{4\pi x} \tag{3}$$

where K_m is the value of K_{III} needed to move the dislocation against τ_p and the image stress. In our current Peierls-Nabarro picture, K_m can be taken to be the critical K_{III} required to convert the core into the planar, mobile state obtainable as the intercepts of the curves at $\Delta = 0$ in Figure 2. In Table 1 are shown these K_m values at various values of x. By fitting eqn. (3) to these data points, we find that τ_p is ~ 0.004μ ahead of a crack tip. The value of τ_p for a dislocation in the bulk can be estimated to be 0.04μ from Figure 3. Thus, a screw dislocation situated in front of a crack tip is predicted to have an effective Peierls stress one order of magnitude lower than if it is situated in a perfect crystal.

TABLE 1
EFFECTIVE PEIERLS STRESS AHEAD OF CRACK TIP FROM PEIERLS-NABARRO MODEL

$\frac{x}{b}$	$\frac{K_m}{\mu\sqrt{b}}$	$\frac{\tau_p}{\mu} = \frac{K_m}{\mu\sqrt{2\pi x}} - \frac{b}{4\pi x}$
3	0.113	~ 0
5	0.107	0.003
10	0.096	0.004

ATOMISTIC SIMULATION

The atomistic simulation was set up by placing a mode III crack plane on a {110} plane with the crack tip parallel to a <111> axis. A ½<111> Burgers vector screw dislocation was also introduced parallel to the same <111> axis on the same {110} plane at a distance x from the crack front. This is similar to the situation in Figure 1. In the MD simulation, an iron-like potential was used and fuller details are given in ref. [10]. The relaxation region was composed of a circular cylindrical crystallite with radius $25a$ (a is the lattice parameter). Periodic boundary conditions were applied along the <111> dislocation direction. In the other two orthogonal directions, the displacement of the boundary region was fixed according to the elasticity solution of the dislocation-crack system.

We have simulated the effects of an applied stress on the core configuration with and without a crack tip in the vicinity of the dislocation. In the crack-free situation without an applied stress, spreading of the core is confined mainly to three intersecting {110} planes. When a shear stress is applied along one of these {110} planes, the spreading on this plane will extend while that on the other two {110} planes will retract. When the configuration is almost planar, the core starts to move. In our simulation, this occurs at a critical applied stress of about 0.027μ, which agrees well with the result reported by Duesbury et al [11] and reasonably well with the value of 0.04μ in Figure 3.

In the presence of a stress-free crack tip, the main effect on the dislocation core is the image force. At distances $x < 5b$ from the crack-tip, because of the large magnitude of the image force, no stable core configuration can be found in our simulation if no applied stress is exerted. For $x \geq 5b$, the dislocation configuration near the unstressed crack tip is similar to that in the bulk but with a negative stress acting. A more or less symmetrical three-fold state as similar to that in the unstressed bulk crystal can however be produced by exerting a positive K_{III} load on the crack so as to counteract the image force. An example of this is shown in Figure 4, which shows the core structure at $x = 8b$. The core spreading configuration at $K_{III} = 0$ (Figure 4(a)) has a turning point on the lower inclining branch and is similar to the structure found

in the crack-free situation with a negative applied shear stress. At $K_{III} = 0.067\,\mu\sqrt{b}$ (Figure 4(b)) the configuration appears very similar to that in the unstressed bulk crystal. The core begins to move at a higher load of $0.170\,\mu\sqrt{b}$. Denoting by K_i the critical load required to completely balance the image force so as to make the core structure appear like that in the unstressed bulk crystal, K_i is given in the Volterra model by

$$\frac{K_i}{\sqrt{2\pi x}} = \frac{\mu b}{4\pi x}. \tag{4}$$

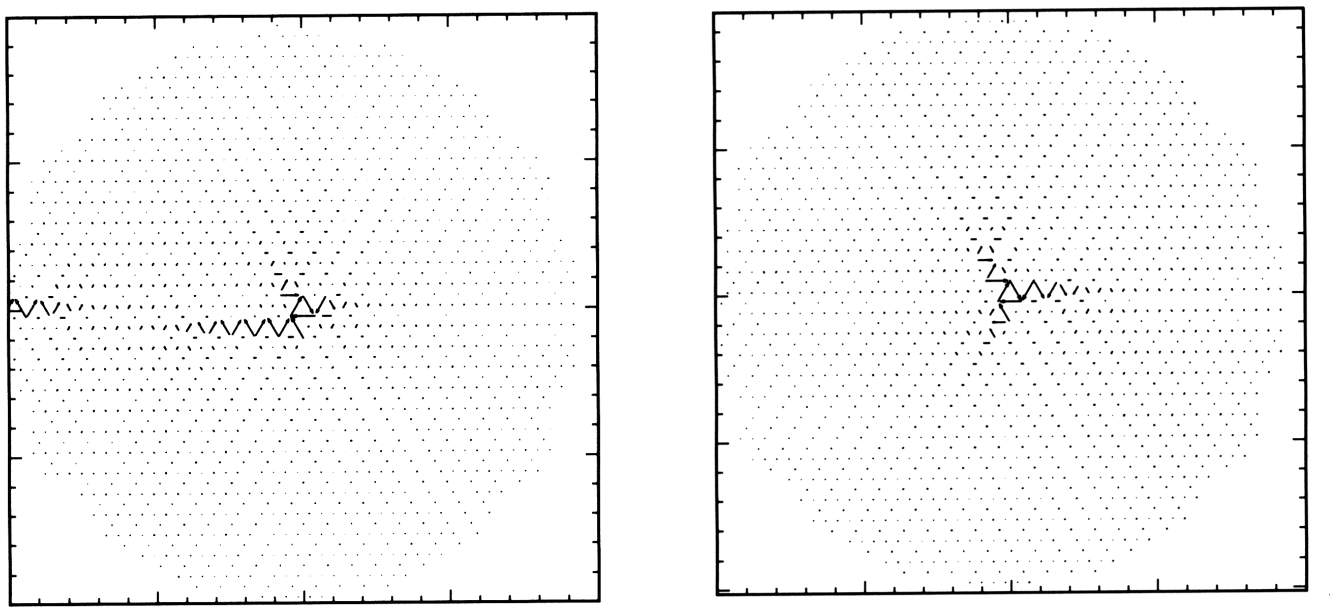

Figure 4: Atomistic core structure when the dislocation is situated at $x = 8b$ from the crack tip. (a) $K_{III} = 0$, (b) $K_{III} = 0.067\,\mu\sqrt{b}$.

Table 2 shows the values of K_i estimated from our atomistic results for $x \geq 5b$. It can be seen that eqn. (4) agrees very well with the atomistic results. This means that at $x \geq 5b$, the crack-tip stress field and the image force can be accurately represented by the elastic K-field and the Volterra dislocation field respectively.

TABLE 2
EFFECTIVE PEIERLS STRESS AHEAD OF CRACK TIP FROM ATOMISTIC SIMULATION

x	"atomistic" K_i $(\mu\sqrt{b})$	$\frac{2\sqrt{2\pi x}\,K_i}{\mu b}$ (= 1 in elastic model eqn. (4))	"atomistic" K_m $(\mu\sqrt{b})$	$\frac{K_m}{\mu\sqrt{2\pi x}} - \frac{b}{4\pi x}$ (= τ_p/μ in elastic model eqn. (3))
$5b$	0.09	1.01	0.15	0.0108
$8b$	0.07	0.99	0.17	0.0140
$12b$	0.06	1.04	0.18	0.0141

The critical load K_m required to move a dislocation core as determined from the atomistic simulation is also listed in Table 2. From the conclusion above, we are confident that the K-term and the image term in eqn. (3) are valid for $x \geq 5b$. The Peierls stress for a dislocation in the bulk crystal is ~ 0.027μ as

mentioned above. However, as can be seen from Table 2, if eqn. (3) is to be obeyed, the effective τ_p ahead of a crack-tip is about 0.014 μ which is only half of the bulk value of 0.027μ. The effective Peierls stress from the atomistic simulation is higher than that calculated from the semi-continuum model in Table 1, but both indicate an enhancement of dislocation mobility ahead of a crack-tip.

DISCUSSION AND CONCLUSION

The semi-continuum results in Figure 2 suggest that the critical load K_m to move the dislocation core decreases slightly as x increases, and that if K_{III} is larger than about 0.12 $\mu\sqrt{b}$, a dislocation that has been freshly emitted from the crack tip (with $x \sim 0$) and all dislocations situated further away would have planar cores and are thus mobile. The atomistic results in Table 2 indicate K_m to be more or less the same at 0.15-0.18 $\mu\sqrt{b}$, which is of similar magnitude as the 0.12 $\mu\sqrt{b}$ from the semi-continuum model. These results therefore suggest the existence of a critical stress intensity factor K_{mc} such that if the applied K_{III} is higher than this value, then all dislocations would be mobile. If the applied K_{III} is lower than K_{mc}, then an immobile zone would exist ahead of the crack tip, the size of which would increase as the difference (K_{mc} - K_{III}) increases. A dislocation situated within this zone would require thermal activation for motion. Rice [5] has suggested the existence of a critical load K_e for dislocation nucleation directly from crack tip and $K_e = \sqrt{2\mu\gamma_{us}}$, where γ_{us} is the unstable stacking fault energy. Taking γ_{us} to be the maximum value of the γ-force law in eqn. (1), $\gamma_{us} = \mu b/(2\pi^2)$, and so $K_e \approx 0.3\ \mu\sqrt{b}$. K_e is therefore of similar magnitude but about one time higher than K_{mc} for motion, implying that nucleation from crack-tip would be more difficult than subsequent motion. Thus, if dislocations can be nucleated from the crack-tip, they should be able to move away from it, implying that crack-tip emission is nucleation rather than mobility controlled.

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